Machine Learning for Deep Trench Bottom Width Measurements using Scatterometry

AM: Advanced Metrology

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Abstract **– We present a machine learning enhanced metrology method to measure the bottom width of deep trenches (about 42 µm in depth) using optical scatterometry. For this study, 2D line trenches as well as circular 3D trenches with varying trench side-wall angles were investigated. A combination of reference sets from SEM cross-sections, inline CD-SEM as well as depth measurements obtained from reflectance fringes are used to train the machine learning model. The results are cross verified against SEM cross-sections.**

Keywords—machine learning, spectral reflectometry, scatterometry, trench shape, bottom CD, CD-SEM, OCD

I. INTRODUCTION

Machine Learning (ML) using optical critical dimension (OCD) or scatterometry metrology has proven itself to be a very powerful tool for inline detection of the geometry of microstructures in the semiconductor industry [1]-[3]. In the case of power devices, be it passive or active components, the control concept for large pitch and deep structures depends on reliable inline detection of trench geometry. Spectroscopic reflectance spectra are useful for obtaining the depth of such trenches. However, modelling the reflectance spectra with traditional Rigorous Coupled Wave Analysis (RCWA) to obtain the bottom width (CD) when the pitch is large, or the trench is very deep, is often quite challenging. In this regard, machine learning based approaches have shown promising results. We show results of one application in this study, where the trenches are about 42 µm deep with a pitch (the distance between trenches) of 6.75 µm. In this case RCWA modeling is not able to accurately obtain the shape (top and bottom critical dimension). Scatterometry, in combination with a ML approach, is then shown to be the way to go. The same is also valid for another application in the form of circular 3D trenches discussed in this study.

A. Scatterometry-based Machine Learning Approach for Trench CD Measurement

In our previous studies, a hybrid metrology method that combines three independent metrology techniques (CD-SEM, mass loss from etching, trench depth measurements from reflectance fringes) was applied to determine a wafer average for the bottom width of deep 42 µm line trench [4]. In this study, a ML approach, investigated on the sister set of wafers, will be presented. This new approach provides additional important information about the wafer uniformity of trench bottom width.

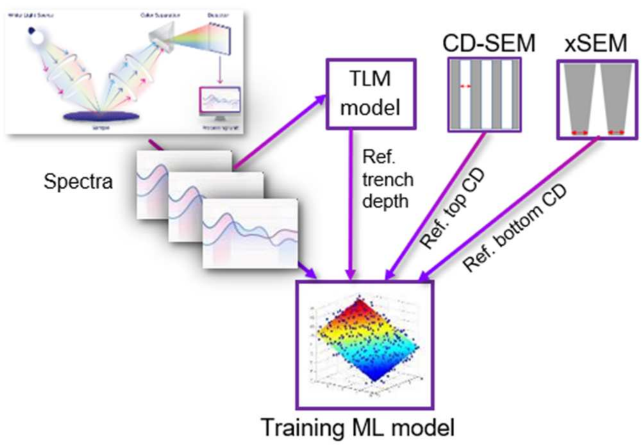


Fig. 1. Machine learning model building scheme.

The reflectance spectra were obtained from a NOVA T600 MMSR tool, which has vertical and oblique incidence advanced scatterometry channels. S-polarized (Rs) and p-polarized (Rp) reflection spectra for the applications below were collected from normal as well as oblique incidence channels with azimuth angles of 0 and 90 degrees. Reflectance spectra were collected from 13 locations on each wafer. The wafers were split into groups (split groups) depending on the etch conditions resulting in varying side-wall angles.

Before applying machine learning methods, it is important to get reference data at the same wafer coordinates where the reflectance spectra were collected. The following reference sets were collected in order to train the ML model. Top widths of the trenches were measured at the same 13 locations with a

CD-SEM after hard mask removal. SEM cross-sections (xSEM) were made to measure bottom widths of the trenches at two locations per wafer, and one wafer from each split group was selected. The trench depths were extracted from the reflectance spectra using NOVA's thick layer measurement (TLM) algorithm [5] and scaled to SEM cross-section reference values.

The ML model was trained using reflectance spectra and reference data for trench bottom widths, top widths and depths. NOVA software was used to build a ML model. The model building scheme is represented in Fig. 1.

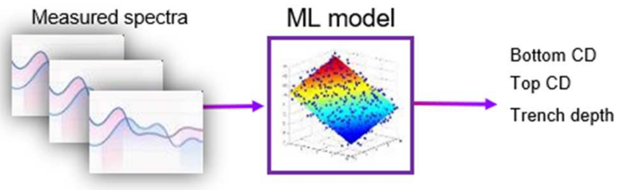


Fig. 2. Machine learning model deployment to obtain parameters of interest from measured spectra.

The trained model is a mathematical estimator, which provides the parameters of interest (POI) - bottom CD, top CD and trench depth, from measured spectra (without reference data) as depicted in Fig. 2. The advantage of such an ML model is that it enables the extraction of weak parameters, i.e. parameters like bottom CD which suffer from low spectral sensitivity in the measurement and cannot be extracted using the classical RCWA approach.

II. Results and Discussion

A. Trench Bottom CD of 2D Line Trenches from ML Method and Comparison with SEM Cross-sections

In the first design of experiment (DOE), five groups of wafers with 2 wafers each were etched in silicon to have different side-wall angles. The first 2 wafers represent the standard process of record (POR). The second and third group received an etch process variation of +/- 3% respectively. The fourth and fifth group had even more deviation in trench side wall angle from POR by changing etch conditions by +/- 8%.

A schematic drawing of 2D line trenches from side view and top view is depicted in Fig. 3.

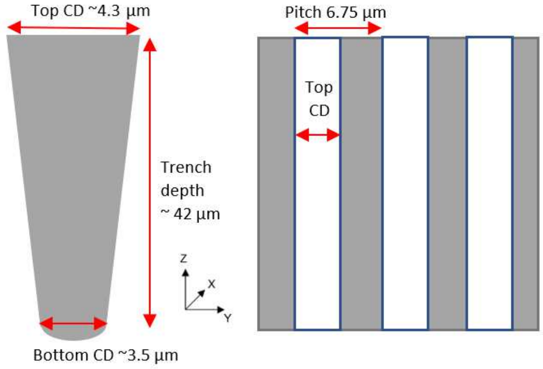


Fig. 3. Schematic image representing side and top view of the 2D line trenches.

Cross-sections were made at right angle through the trenches at two positions per wafer (center and wafer edge) and were used as reference bottom CD data for ML model training. One wafer from each split group was cross sectioned which gives in total 10 reference data. Top widths of the trenches were measured using a CD-SEM tool and used as reference data. Scatterometry spectra were collected at the same wafer locations as for SEM cross-sections and CD-SEM measurements. The reference trench depths were extracted from reflectance spectra using the thick layer measurement algorithm and scaled to SEM cross-section reference values. The ML model was trained using scatterometry spectra and reference data for bottom CD, top CD, and trench depth from SEM cross-sections, CD-SEM, and TLM model, respectively.

Fig. 4 shows a radial profile of ML model predicted bottom CD values (small symbols) together with SEM cross-section reference values (large symbols, used in the training set). The solid lines are spline fits to the bottom CD data obtained with the ML method. The symbols and line in red indicate the measurement data from the wafer etched with POR condition. The results from wafers with BCD +, BCD ++ and BCD-, BCD-- etch conditions are observed above and below the POR wafer respectively. Not only is the split in the bottom CD clearly distinguishable, but also a similar radial trend for each wafer is obtained. Two of the 13 measured points have nearly the same bottom CD as the cross-section reference and are therefore covered by the larger cross-section symbols in Fig. 4.

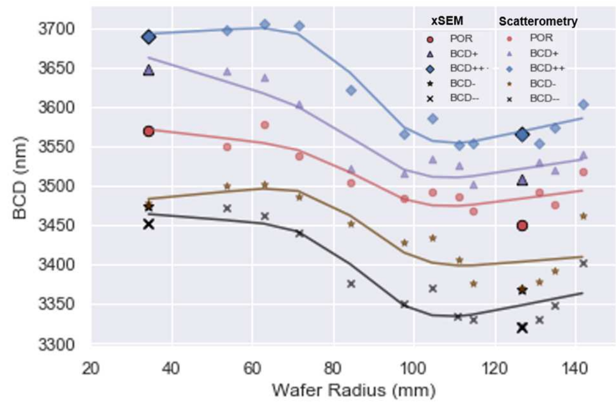


Fig. 4. Bottom CD of line trenches as a function of wafer radius. The larger symbols at 35 and 125mm radius are reference data from SEM cross-sections (used in the training set). The smaller symbols are the results from the scatterometry measurements using ML. The solid lines are spline fits to the bottom CD data obtained with the ML method.

The performed Leave-One-Out Cross-Validation (LOOCV), by leaving one reference data point out, gave good correlation of ML model predicted values (R^2=0.96) with reference SEM cross-section bottom CD values. Cross-validation is used with the aim to estimate the performance of the machine learning algorithm by predicting data not used in the training of the model. LOOCV uses the following approach to evaluate the ML model. The data set is split in a training set and a testing set. For example, there are 10 reference data points. One reference data point is "left out" from the training set and the remaining 9 reference points are used for the ML model training. The trained model predicts the value for the one reference point that was left out. The procedure is repeated 10 times by leaving out different reference points.

Besides bottom CD, the top CD as well as depths of the trenches were obtained using the same ML model. This implies, in production, all the geometric parameters can be obtained in the same measurement operation. However, the LOOCV was used only for the bottom CD and not for the depth or top CD.

In order to have a better comparison as well as visualization, the POR wafer (same POR wafer as presented in Fig. 4) had a full-wafer measurement of top CD with CD-SEM (97 sampling points) and scatterometry using the ML model (107 sampling points). The top CD and trench depths agree with CD-SEM and SEM cross-sections reference data as shown in Fig. 5 and Fig. 6, respectively. The uniformity across the wafers is as expected for the etch process. Top CD of line tranches decreases from wafer center, reaches plateau at 80-120 mm wafer radius, and starts increasing again toward the wafer edge, as observed in Fig. 5. Line trench depth increases from wafer center to edge, as shown in Fig. 6.

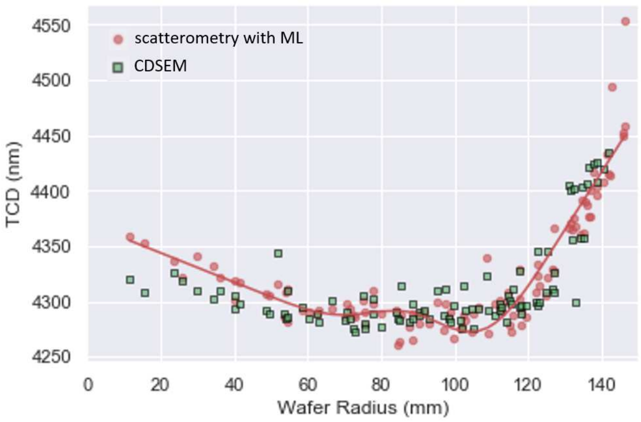


Fig. 5. Top CD of the line trench POR wafer as a function of wafer radius, comparing CD-SEM (green square symbols) and scatterometry measurements using the ML method (red circles).

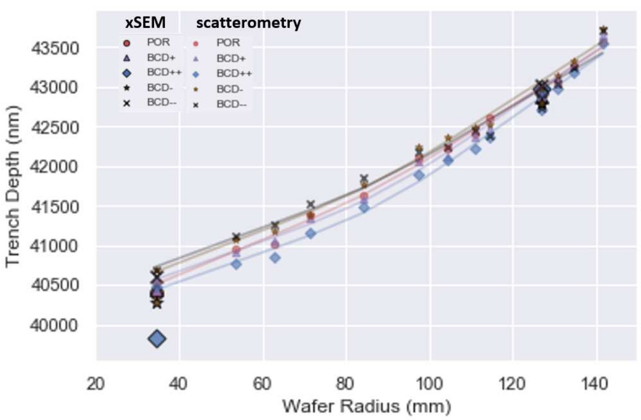


Fig. 6. Depth of line trenches as a function of wafer radius. The larger symbols at 35 and 125mm radius are data from SEM cross-sections. The smaller symbols are the results from the scatterometry measurements using ML. The solid lines are spline fits to the obtained trench depth data from scatterometry measurements using the ML method.

In order to verify the above developed model, scatterometry measurements were performed on an independent lot with 25 productive wafers, which were not part of the training set. The results obtained are discussed in the following section.

Full-wafer maps and radial profiles of productive wafers, obtained from scatterometry measurements with the ML model, are shown in Fig. 7 and Fig. 8, respectively. The contour plots (Fig. 7) of bottom CD (a), trench depth (b), and top CD (c) are based on 107 measurement points and reveal a radial symmetry for these trench properties. The bottom CD, trench depth and top CD radial profiles for 3 productive wafers (Fig. 8) are comparable to the POR wafer radial profiles of Fig. 4, Fig. 5 and Fig. 6 that were used in the training set. Bottom CDs reach highest values at ~50 mm wafer radius and lowest values at 100-120 mm radius, as can be observed in Fig. 8 (a).

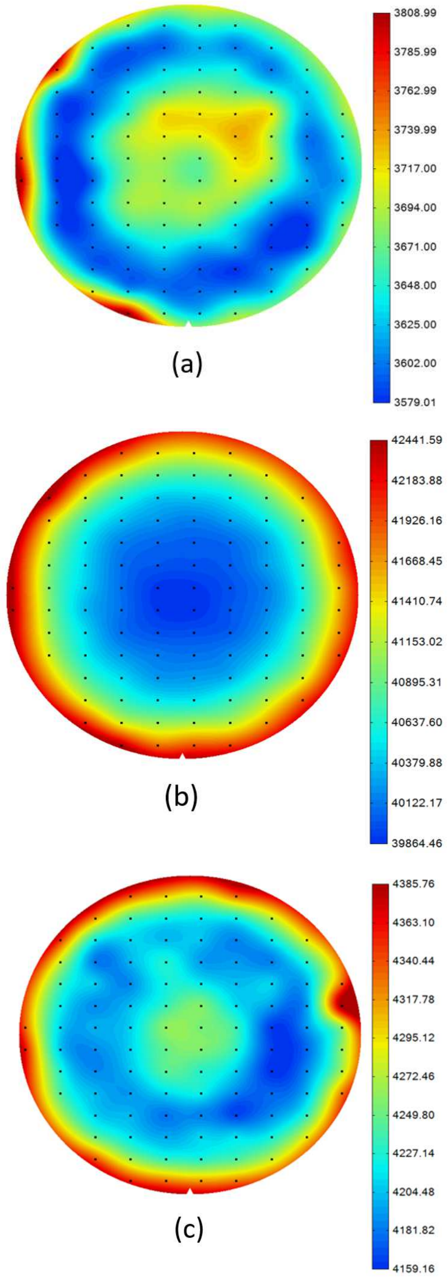
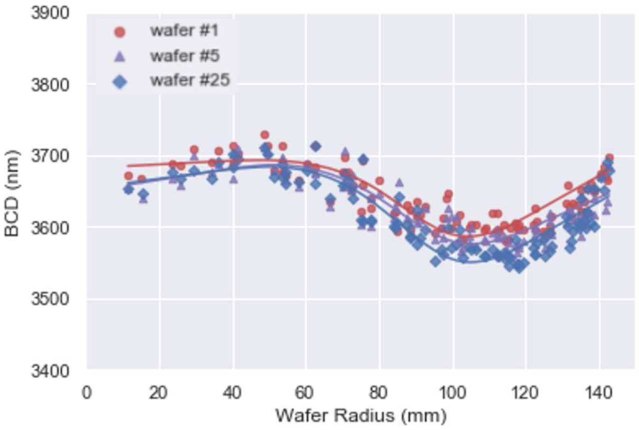
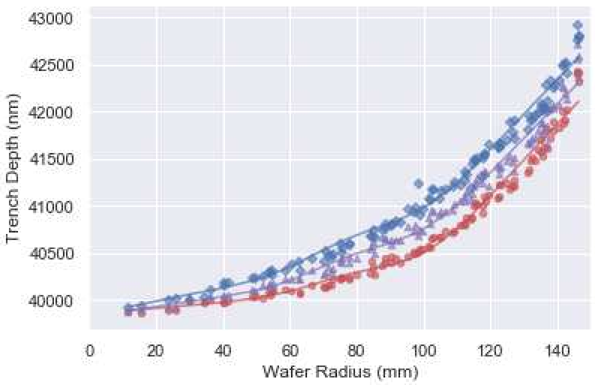


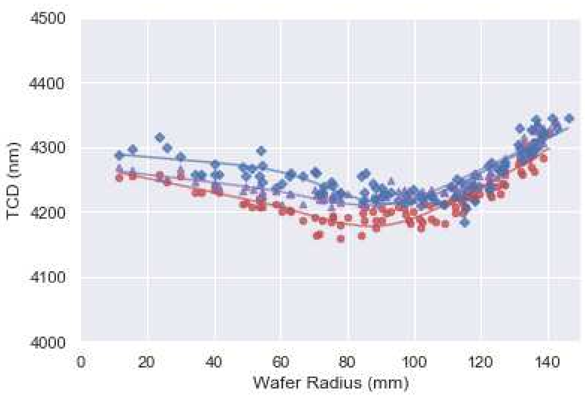
Fig. 7. Wafer maps for productive wafer #1 with line trenches. (a) bottom CD, (b) trench depth, and (c) top CD obtained from scatterometry measurements using the ML method. Numerical values are in nanometers. This productive wafer was not used in the training set.



(a)



(b)



(c)

Fig. 8. Radial profile for productive wafers #1, #5, and #25 of (a) bottom CD, (b) trench depth and (c) top CD obtained from scatterometry measurements using the ML method. These wafers with linear trenches were not used in the training set.

Similar to the goodness of fit in the RCWA based approach, a confidence index is also available to test the applicability of the developed ML model. Out of the set of 25 POR wafers, fliers in bottom CD were observed in three wafers (not shown here), at different locations on each wafer. At the same locations, the confidence index dropped to about 40% of the maximum value. Further investigation was carried out by comparing the measured spectra (from multiple scatterometry channels) with low and high confidence index values. Indeed, the spectra at the positions with low confidence index were very different from the ones at positions with high confidence index and outside the set of spectra used for training the ML model. Additionally, optical defect inspection was carried out for all 25 wafers. From these defect density wafer-maps, those locations were singled out where lower confidence indices in trench measurement were observed. At those locations with low confidence index, dense clusters of defects were observed. Defects in the measurement area have a strong effect on the recorded spectra and lead to considerable reduction in the confidence index. The nature of the defect is out of the scope of this paper however, it suffices to state that the ML model is sensitive enough to detect any deviation from the permitted trench geometry. As a next step, the model will be tested in volume production and monitored for any possible drifts of the model.

B. Trench Bottom CD of 3D Circular Trenches from ML Method and Comparison with SEM Cross-sections

As a second example, we present results from circular trenches that were etched (> 7 µm deep) in 300 mm silicon wafers. Fig. 9 shows schematically the top as well as the side-view of the 3D trenches. The trenches had an aspect ratio of width to depth of about 1:4. Such an aspect ratio proved to be challenging for the measurement of bottom CD, using the traditional RCWA method only, owing to the small signal amplitude of the reflectance spectra. Therefore, the ML method was used in combination with scatterometry to measure the bottom CD of the circular trenches. As part of the DOE, seven groups with different etch conditions were prepared with two wafers in each group. Again, the first group represents POR wafers. The second and fourth group received an etch process variation of +/- 3% respectively. The third and fifth group had even more deviation in trench side wall angle from POR by changing etch conditions by +/- 6%. The final two groups underwent top CD variation lithographically by up to +/- 2%.

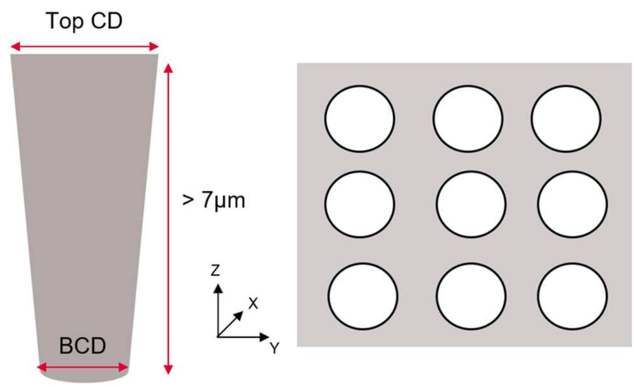


Fig. 9. Schematic images representing side as well as top view of the 3D circular trenches.

Cross-sections were made at right angle through the circular trenches at two positions per wafer (from center and wafer edge) and were used to obtain reference data for bottom CD. One wafer from each group was cross sectioned which yielded in total 14 reference data. Top widths of the circular trenches were measured using a CD-SEM tool and used as reference data. Scatterometry spectra were collected at the same wafer locations where SEM cross-section and CD-SEM measurements were made. The thick layer measurement algorithm was used to get reference trench depths from reflectance spectra after scaling to SEM cross-section reference images.

The machine learning model was trained using scatterometry spectra and reference data for bottom CD, top CD and trench depth from SEM cross-sections, CD-SEM and TLM model, respectively. Using the ML approach, it was possible to obtain circular trench depth, top CD as well as bottom CD. The normalized bottom CDs from 14 cross-sections are plotted versus bottom CDs obtained with the ML method (Fig. 10). The performed Leave-One-Out Cross-Validation (LOOCV), by leaving one reference data point out, gave ML model predicted values which have a good correlation (R^2=0.91) with reference SEM cross-section bottom CD data (Fig. 10).

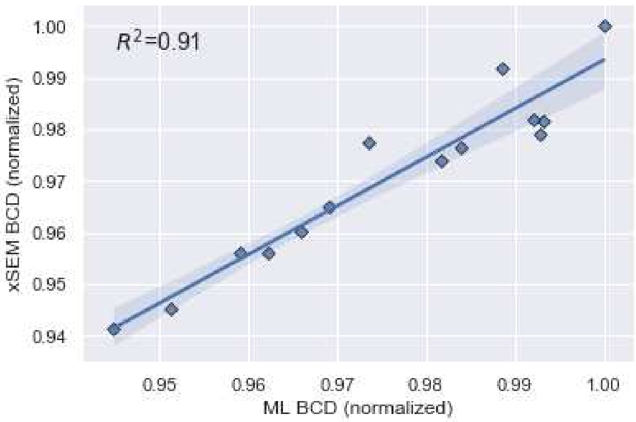


Fig. 10. Circular trench bottom CDs obtained from cross-sections are plotted versus values obtained from Leave-One-Out Cross-Validation (LOOCV). 14 cross-sections were made from the split group of 7 wafers.

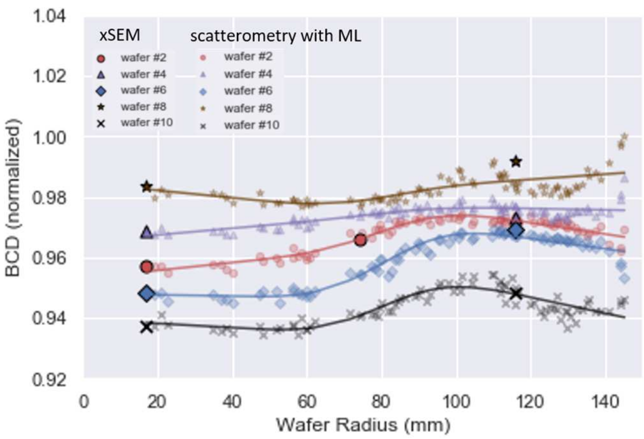


Fig. 11. Bottom CD of circular trenches as a function of wafer radius. The larger symbols at 17, 74 and 116 mm radius are reference data from SEM cross-sections (used in the training set). The smaller symbols are the results from the scatterometry measurements using ML. The solid lines are spline fits to the bottom CD data obtained with the ML method.

Fig. 11 shows the radial profile plot of circular trench bottom CD for 5 wafers, which had a bottom CD variation. The small symbols represent the measured bottom CD using ML and the line is a spline fit to the measured data (87 sampling points per wafer). The symbols in red represent the measurement from wafer #2 with POR condition. The bottom CD from wafers #4 and #6 with +/-3% process variation, respectively, are observed to lie just above and below the POR wafer (#2). The +/-6% process variation (wafers #8 and #10) brings the measurement data even further away from the POR wafer. However, the radial profiles of all the wafers are similar to each other. The big symbols represent SEM cross-section data from wafer center and edge and good agreement with measured bottom CD is observed for all the wafers.

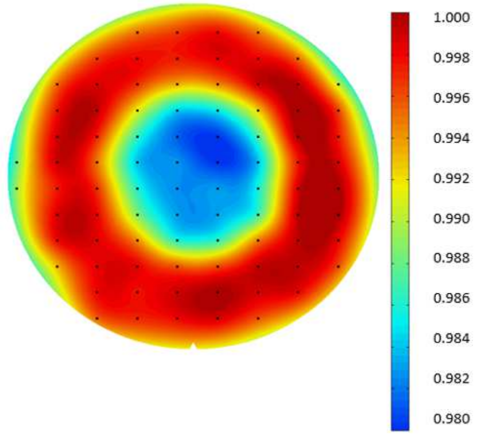


Fig. 12. Wafer map of bottom CD for circular trenches of the POR wafer (normalized values) obtained from scatterometry measurements using an ML model.

Full-wafer map measurements of bottom CD, obtained from scatterometry with the ML model, are shown in Fig. 12. The bottom CD for circular trenches of the POR wafer has a radially symmetric pattern. In the contour plot the bottom CD is lowest in the wafer center and increases with increasing radius up to 105mm. Between 105 and 145mm radius bottom CD decreases again slightly (Fig. 12).

The ML model was trained using CD-SEM reference data for top CD and TLM model reference data for trench depth. SEM cross-section measurements were used for testing the model. The cross-sections were done at the same wafer locations as scatterometry measurements. One measurement point out of 14 SEM cross-section measurement points was removed, because it was identified as an outlier.

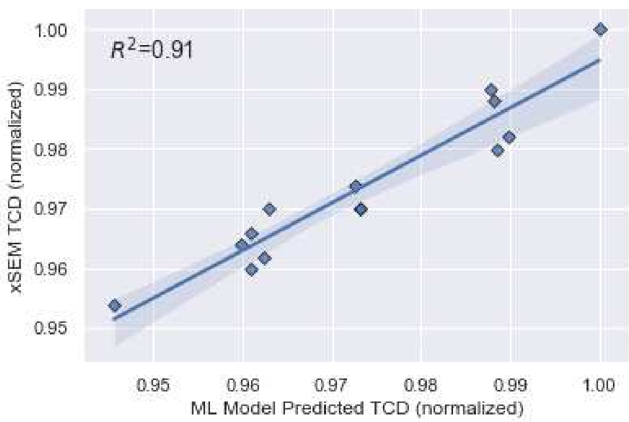


Fig. 13. Circular trench top CD measured in SEM cross-sections is plotted versus scatterometry measurements using the ML method. The SEM cross-section data were not used in the training set.

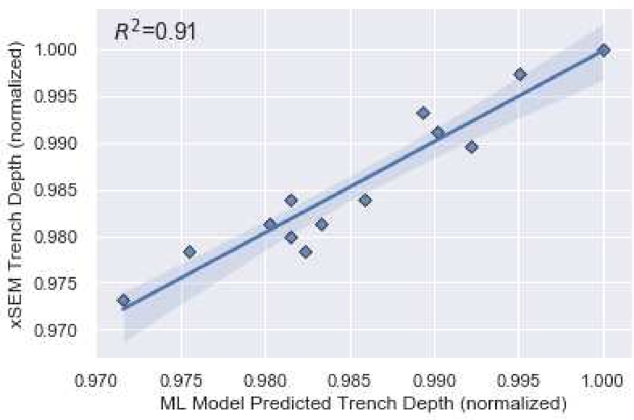


Fig. 14. Circular trench depth obtained from SEM cross-sections is plotted versus scatterometry results using the ML method. The SEM cross-section data were not used in the training set.

The top CD as well as depth, measured with the scatterometry based ML model, agree well with the SEM cross-section data (not used in the training set), with a correlation $R^2 = 0.91$. Fig. 13 and Fig. 14 show correlation plots for top CD and depth of the circular trenches, respectively, obtained from scatterometry using an ML model and SEM cross-section reference data that were not used in the training set.

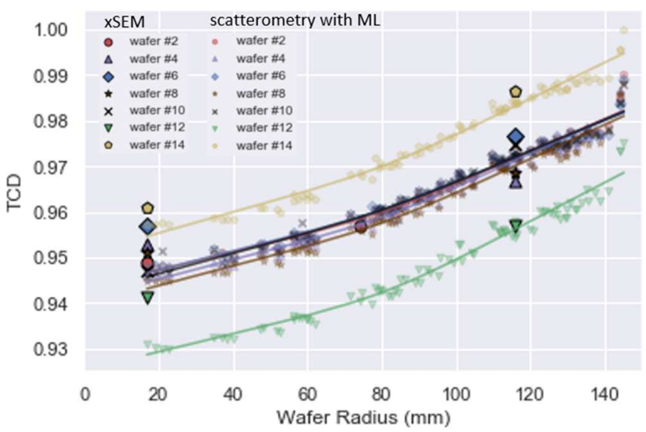


Fig. 15. Top CD (normalized) of circular trenches as a function of wafer radius. The larger symbols at 17, 74 and 116 mm radius are reference data from SEM cross-sections (not used in the training set). CD-SEM data were used for training the ML model. The smaller symbols are the results from the scatterometry measurements using ML. The solid lines are spline fit to the obtained bottom CD data from the ML method.

Additionally, the radial profile plot for circular trench top CD is shown in Fig. 15. The top CD for wafers #2 - #10 was not affected by the variation in bottom CD. The data for the two wafers (#12 and #14), which underwent top CD variation lithographically, are observed to be split above and below the cluster of wafers #2 - #10. The radial profile of top CD is similar for all wafers increasing from wafer center towards the edge.

III. Summary and Conclusions

Scatterometry measurements, using a machine learning approach, enabled us to extract bottom CDs for deep line trenches (2D) and circular (3D) trenches in silicon. Good agreement with reference SEM cross-sections for bottom CD was obtained. The machine learning approach is particularly useful in cases where RCWA modelling is not able to extract information about the width of trenches at the bottom. Moreover, the combination of scatterometry measurements with machine learning can provide much-desired wafer uniformity information for the bottom CD of deep trenches.

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